REPORT DOCUMENTATION

Form Approved
OMB No. 0704-0188

AFRL-SR-AR-TR-02-
0277

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
22-07-2002	Final Report	01-04-2001 to 31-03-2002

4. TITLE AND SUBTITLE
Quantitative Visualization of Turbulent Reactive Flows in Propulsion Systems

5a. CONTRACT NUMBER

5b. GRANT NUMBER
F49620-01-1-0200

5c. PROGRAM ELEMENT NUMBER
61103D

6. AUTHOR(S)
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5d. PROJECT NUMBER
3484

5e. TASK NUMBER
US

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR
801 North Randolph Street
Room 732
Arlington, VA 22203-1977

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release, distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT
A computational/graphical engine and graphic software were purchased. These items were used extensively in our AFOSR sponsored research on large eddy simulation (LES) of turbulent reacting flows. In particular, they were utilized for quantitative visualization of the unsteady flow features as predicted by LES of several flow configurations.

20020909 147

15. SUBJECT TERMS
Flow visualization, large eddy simulation, turbulent combustion, subgrid scale modeling.

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
					Julian M. Tishkoff
a. REPORT	b. ABSTRACT	c. THIS PAGE	UL	8	19b. TELEPHONE NUMBER (include area code)
unclassified	unclassified	unclassified			(703) 696-8478

QUANTITATIVE VISUALIZATION OF TURBULENT REACTIVE FLOWS IN PROPULSION SYSTEMS

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Abstract

Under the support of this program, a computational/graphical engine and a graphic software were purchased. These items were used extensively in our AFOSR sponsored research on large eddy simulation (LES) of turbulent reacting flows. In particular, they were utilized for quantitative visualization of the unsteady flow features as predicted by LES of several flow configurations. The simulations were based on our recently developed filtered density function (FDF) methodology, in which the FDF transport equation was solved via a Lagrangian Monte Carlo scheme. All computations and the subsequent quantitative flow visualizations were performed exclusively on this engine. Excellent run times were obtained with user-friendly graphical post-processing of data.

Equipment

With the DURIP support, we purchased the following equipment:

- **SUN Fire 4800:** This is a 64-bit computing engine which is a powerful tool for computation and for graphics when used in conjunction with a graphic software. This shared-memory supercomputer uses twelve 900 Mhz UltrSPARC III (Super-scalar SPARK v9) processors with 8 MB of e-cache per processor and 24 GB of memory (expandable to 96 GB) to deliver top computing performance. The server contains three four processor modules connected via SUN Fireplane and capable of sustained 9.6 GB data transfer rate. The local storage is provided via SUN StorEdge D240 media tray containing two 18.2 GB using dual-channel differential UltraSCSI adapter, a DVD-ROM drive and a DDS-4 tape drive. SUN Fire 4800 is powered by SUN's state of the art Solaris Operating Environment version 8. An estimated cost of this supercomputer reaches upward of U.S. $500,000 ($520,785 as configured above). Additional information about SUN Fire series of servers can be found at the web site:`http://www.sun.com/servers/midrange/`

- **Tecplot:** Complementing our computation, we purchased this state-of-the-art and widely accepted visualization software. Tecplot is produced and licensed by Amtec Engineering, Inc. It allows for efficient visualization and analysis of data via multitude of built-in macros and functions. In Spring 2002, a single-user perpetual license cost U.S. $1,497.50. Additional information about Tecplot software can be found at the web site:
`http://www.amtec.com/Product_pages/tecplot9/`

In our original proposal, we requested to purchase an ONYX2 engine from SGI (Silicon Graphics, Inc.) However, at the time of purchase, the SGI was no longer under the New York State contact with our University. Therefore, it would have been impossible for us to maintain this engine in our laboratory for an extended period of time. Therefore we decided to purchase the SUN 4800 server. This decision proved extremely fruitful as the equipment as purchased provided excellent supercomputational/graphics capabilities in our AFOSR sponsored research.

Utilization of Equipment

The main thrust of current research is sponsored by the Air Force Office of Scientific Research under Grant F49620-00-1-0035. This research is entitled: "Filtered Mass Density Function for Subgrid Scale Modeling of Turbulent Diffusion Flames." Dr. Julian M. Tishkoff is the Technical Monitor of this Grant. We are also involved in two other sponsored research programs: The first involves numerical simulation of supersonic reacting flows. This work is sponsored by the NASA Langley Research Center (Grant NAG-1-1122). The second involves numerical simulation of gravity effects in transitional and turbulent diffusion flames. This work is sponsored by the Microgravity Science Division of the NASA Headquarters and is administrated by the NASA Glenn Research Center (Grant NAG-3-2225).

The equipment as purchased was used extensively in our AFOSR sponsored project in large eddy simulation (LES) of turbulent reacting flows. This approach is considered somewhere between direct numerical simulation (DNS) and Reynolds averaged simulations (RAS).[1–3] Over the past thirty years since the early work of Smagorinsky[4] there has been relatively little effort, compared to that in RAS to make full use of LES for engineering applications. The most prominent model has been the Smagorinsky eddy viscosity based closure which relates the unknown subgrid scale (SGS) Reynolds stresses to the local large scale rate of flow strain. The extensions to "dynamic" models[5] have shown some improvements. This is particularly the case in transitional flow simulations where the dynamic evolutions of the empirical model "constant" result in (somewhat) better predictions of the large scale flow features.[6]

We have recently developed a methodology which has proven very effective for modeling of the SGS fluctuations in turbulent reacting flows. The methodology is termed the "filtered density function" (FDF),[7–10] and is based on the idea of representing the effects of SGS fluctuations in a "probabilistic" manner, and simulating the large scale transport deterministically. The FDF is essentially the probability density function (PDF) of the SGS quantities. Thus, it has all the capabilities of PDF methods as widely recognized in RAS.[11] Several "simple" means of implementing the methodology based on the "assumed" PDF of SGS scalars have also been reported.[12–16] However, it has been only recently that we[7–10] have been able to derive a "transport equation" for

the evolution of the FDF and to solve this equation in a "mathematically-consistent" and "computationally-efficient" manner. In this transport equation, the effects of chemical reactions on the SGS statistics appear in a *closed form*, allowing reliable LES of turbulent combustion.

High speed computer graphics constitute an integral part of our efforts in LES/FDF. Because of the added dimensionality of the compositional variables, the "Lagrangian Monte Carlo" scheme[17] provides the most efficient means of simulating the FDF. This scheme has proven effective in RAS;[11] and we have been successful in its utilization for LES. To demonstrate the importance of quantitative flow visualization in LES/FDF, the contour plots of the particle number density of the Monte Carlo particles in LES of a three dimensional flame is presented in Fig. 1. This number density is highly correlated with the (first moment of the) filtered fluid density. This correlation is necessary to ensure that the physics of the problem is correctly captured by the simulations. It is of crucial importance to keep track of the number density, including the locations of all the Lagrangian particles at all times as the simulations proceed. This is a very challenging data management task. With integration of the Monte Carlo data, the filtered variables are readily determined. For example, Fig. 2 shows the convolution of the flame surface at an instant of (frozen) time.

In closure of this report, we would like to state that since our early work on FDF, this methodology has been used by several other investigators;[18–20] See Ref.[21] for a recent review. Quantitative visualization plays a major role in complementing our large scale simulation via FDF. The equipment as purchased under the support of this program helped significantly in these efforts and will remain an integral part of our future activities.

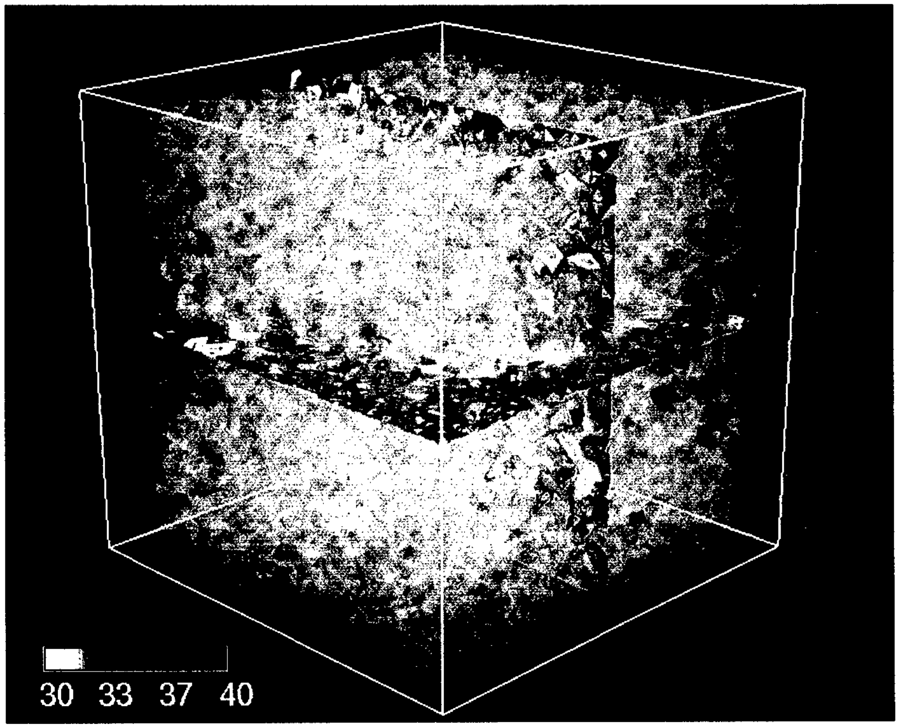

Figure 1. Monte Carlo particle number density in a turbulent flame

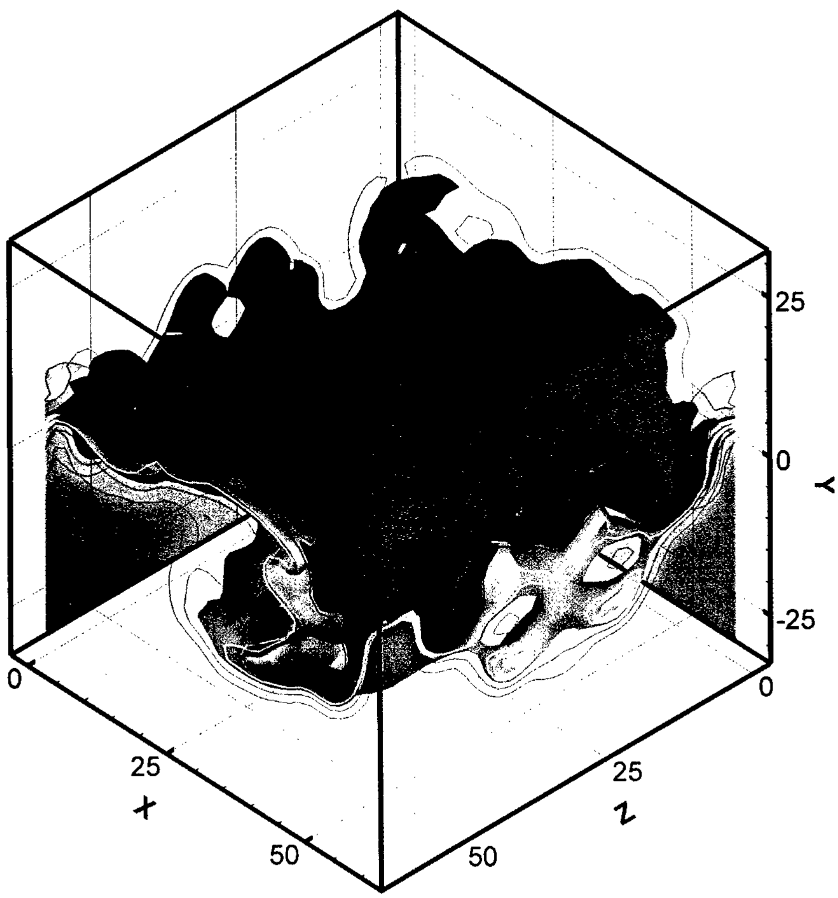

Figure 2. Topology of the flame surface as obtained by LES/FDF

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